Pacifigorgia-1(9),10-diene

Inchi: InChI=1S/C15H24/c1-10(2)9-15-12(4)5-7-13-11(3)6-8-14(13)15/h8-9,11-13,15H,5-7H2,1-
InchiKey: DMSFMSTWAVYMQU-CZPDGURSSA-N
Formula: C15H24
SMILES: CC(C)=CC1C2=CCC(C)C2CCC1C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	237.20	kJ/mol	Joback Method
hf	-112.75	kJ/mol	Joback Method
hfus	26.44	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1383.80		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1384.00		NIST Webbook
tb	567.73	K	Joback Method
tc	781.26	K	Joback Method
tf	269.89	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.02	J/mol×K	567.73	Joback Method
cpg	525.17	J/mol×K	603.32	Joback Method
cpg	546.96	J/mol×K	638.91	Joback Method
cpg	567.45	J/mol×K	674.49	Joback Method
cpg	586.71	J/mol×K	710.08	Joback Method
cpg	604.80	J/mol×K	745.67	Joback Method

cpg	621.79	J/mol×K	781.26	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R332091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume